

Toward general solutions to time-series problems: Notes on obstacles and noise

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Abstract

Computational difficulties in the general application of Bretthorsts formalism to time-series problems, posed by the large number of possible models and the use of models with nonorthogonal base-functions are discussed. The specific problem under consideration is a Bayesian procedure for model selection, parameter estimation, and classification, that was applied to the search for the *In Vivo* T_2 decay rate distributions in brain tissues. Through the estimation of the meta-parameter σ in the process, we also gain a better understanding of the meaning and estimation of "noise" in the frame-work of probability theory as logic.

1 Introduction

Probability theory as logic establish the unique procedure with which one can find the probability assignment to any well-posed inference problem. Nonetheless, this procedure may still be difficult to compute. In [1], Bretthorst present a mathematical frame-work in which time-series problems can be treated: In this frame-work, Each of our models is a linear combination of base functions. that is, the model M_α as a function of the time t , is of the form:

$$M_\alpha(t) = \sum_{j=1}^{m_\alpha} B_{j\alpha} G_{j\alpha}(t, \vec{\tau}_{j\alpha}) \quad (1)$$

Where:

- $\vec{\tau}_{j\alpha}$ is the set of the nonlinear parameters of the base function $G_{j\alpha}$.
- m_α is the number of base functions appearing in model α .
- $B_{j\alpha}$ is the amplitude of base function $G_{j\alpha}$.

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The measurements are described by:

$$d_l = M_\alpha(t_l) + e_l$$

where e_l is the noise realized in measurement l . Given the model and a parameter set, the difference between a datum value and the value (of this datum) predicted by the model is assigned to the noise.

We discuss here the case of Gaussian assignment to the noise, and discuss the arising computational implications. Indeed, the assignment of Gaussian probability distribution to the noise is a special case, but a very important one: arising from maximum entropy considerations, it is the proper encoding of our ignorance regarding non-systematic effects with known/finite variance [4].

The probability of getting the value of a datum point, given the Gaussian probability distribution of the noise, its variance σ_s , and all the model parameters, is:

$$p(d_l/\vec{B}_\alpha \vec{\tau}_\alpha M_\alpha \sigma_s I) = \frac{1}{\sqrt{2\pi\sigma_s^2}} \exp\left(-\frac{1}{2\sigma_s^2} \left(d_l - \sum_{j=1}^m B_{j\alpha} G_{j\alpha}(t_l, \vec{\tau}_{j\alpha})\right)^2\right)$$

For the sake of clarity, from now on we omit the index α that signified the model M_α and the explicit symbol of the model M_α . We do everything inside the model under consideration.

We deal with the general case of multiple measurements. That is, each time-series was sampled more than once. The noise is assumed uncorrelated, and thus the probability of getting this data is the product of the probability of getting each of the data points:

$$\begin{aligned} p(D/\vec{\tau} \vec{B} \sigma_s I) &= \prod_i^n \prod_l^{n_l} p(d_{il}/\vec{\tau} \vec{B} \sigma_s I) \\ &= (2\pi\sigma_s^2)^{-\frac{n \cdot n_l}{2}} \exp\left(-\frac{1}{2\sigma_s^2} \sum_{i=1}^n \sum_{l=1}^{n_l} (d_{il} - \sum_{j=1}^m B_j G_j(t_i, \vec{\tau}_j))^2\right) = \\ &= (2\pi\sigma_s^2)^{-\frac{n \cdot n_l}{2}} \exp\left(-\frac{Q}{2\sigma_s^2}\right) \end{aligned} \quad (2)$$

Where

$$\begin{aligned} Q &= nn_l \vec{d}^2 - 2 \sum_{j=1}^m \sum_{i=1}^n B_j G_j(t_i, \vec{\tau}_j) \cdot \sum_{l=1}^{n_l} d_{il} + n_l \sum_{j=1}^m \sum_{k=1}^m g_{jk} B_j B_k \\ g_{jk} &= \sum_{i=1}^n G_j(t_i, \vec{\tau}_j) \cdot G_k(t_i, \vec{\tau}_j) \end{aligned}$$

$$\overline{d^2} = \frac{1}{n \cdot n_l} \sum_{i=1}^n \sum_{l=1}^{n_l} d_{il}^2$$

and

- m – Number of model base functions.
- n – Number of sampling points.
- n_l – Number of measurements of each time-series

Equation (2) is the key expression to be computed in any calculation of probabilities in time series problems with Gaussian noise.

In order to understand the implications of having multiple measurements and the relationship between the part of noise arising from the misfits of the data to the model and the part of noise arising from the non-systematic effects, we let:

$$\sigma^2 = \frac{\sigma_s^2}{n_l}$$

and use this quantity from now on. So,

$$p(D/\vec{\tau} \vec{B} \sigma I) = (2\pi n_l \sigma^2)^{-\frac{n \cdot n_l}{2}} \exp\left(-\frac{Q}{2\sigma^2}\right) \quad (3)$$

$$Q = n\overline{d^2} - 2 \sum_{j=1}^m \sum_{i=1}^n B_j G_j(t_i, \vec{\tau}_j) \overline{d_i} + \sum_{j=1}^m \sum_{k=1}^m g_{jk} B_j B_k$$

Where:

$$\overline{d_i} = \frac{1}{n_l} \sum_{l=1}^{n_l} d_{il}$$

We see that $\overline{d_i}$, the average of the data points for every sampling time i , is sufficient for finding the maximum of the likelihood. It is not sufficient to establish the absolute value of the likelihood at any point of the parameter space.

Nevertheless, in case σ is known, $\overline{d_i}$ is sufficient for any calculation of the parameters' values, since the likelihood dependence on the more detailed distribution of the data is through a constant factor, $\overline{d^2}$.

As common sense suggests, if σ is unknown, the extent to which the data points are distributed will determine the probability distribution of σ . The probability distribution of σ , in turn, will not influence the values of the parameters at maximum likelihood, but will determine the width of the likelihood and of the probability distributions for the parameters.

In order to compute the probability of the model $P(M/DI)$ for the model comparison and estimation of the parameters, one must integrate the likelihood given in Equation(3) over all the model parameters.

Having the base functions orthogonal, in the sense that:

$$g_{jk} = \sum_{i=1}^n G_j(t_i) \cdot G_k(t_i) = \delta_{jk}$$

will enable us to analytically integrate the likelihood over the linear parameters. Moreover, in case the base functions are orthonormal, the expectation values of their amplitudes are given directly by the projection of the data on the base functions [1].

In spite of the general dependence of the base functions on nonlinear parameters, the base functions will be, in many important problems, almost orthogonal. For example, in the problem of evenly sampled multiple stationary frequencies, with cosines and sines as the base functions, the off diagonal terms of g_{jk} will be negligible as long as the frequencies are well separated [1].

In this paper we demonstrate the application of Bretthorsts' formulation for a rather pathological problem, in which the matrix g_{jk} is never orthogonal. The computational difficulties, arising from the existence of nonlinear parameters in our problem, lead us to consider computation-reduction tools:

First, arranging the models into a multi-dimensional model space, in which a search can be performed instead of impractical calculation of the probability of all the models. Second, the Bretthorst formulation teach us how to analytically integrate over the linear parameters, but we still have to integrate over the nonlinear parameters numerically or through approximations. Numerical integrations are usually impractical in spaces of many nonlinear parameters. We are left with the task of finding the transformation of the likelihood (as a function of the nonlinear parameters) into forms that can be approximated with satisfactory precision.

Analyzing a multiple-measurements problem, we also note about the "noise" and its meaning in the Bayesian framework. In cases of multiple-measurements, we can rarely estimate the noise by using statistics like the Standard Deviation.

2 Posing the Problem

2.1 The Data

Using a 32 echo CPMG MR imaging sequence on a 1.5T GE clinical MR scanner, spin-spin relaxation (T_2) decay curves were acquired from the brains of 11 normal humans [6]. A decay curve is the collection of the amplitudes of the same pixel in the image through 32 consecutive images. Accordingly, each decay curve contains amplitudes of 32 points in time, from 10 to 320ms (Figure (1)). The partition to specific tissues was assigned by a neurologist on the images of

Figure 1: Sample of the Raw Data. Different symbols signify data taken from different humans.

ten brains. For each of twelve tissues, five of white matter and seven of gray matter, 800-5000 decay curves had been collected. The eleventh brain's data provides the new data for the classification stage.

It is clear from the Bayesian standpoint, that we lose information by using this data instead of the raw signal collected by the scanner. The available data is the result of the imaging reconstruction, including FFT, and thus suffers from FFT artifacts. Moreover, after assigning the specific tissues, the localization of the pixels' data is lost, preventing us from taking possible tissue assignment errors and inter-tissue contamination into account. Nevertheless, in our formulation of the problem, we regard this data as the raw data. The information loss will contribute to the "noise".

2.2 Background Information

2.2.1 The Set of Models

The mechanism that produced the decay curves is modeled by:

$$d_i = \int_0^\infty f(T_2) \cdot e^{-\frac{t_i}{T_2}} dT_2 + [a + [bt + [ct^2]]] + d \cdot (-1)^i \cdot e^{-\frac{t_i}{T_0}} + Noise$$

Where $i=1..32$

- The T_2 Distribution $f(T_2)$ is expected to be composed of a few discrete components. These components are parameterized by their amplitude,

Figure 2: Example of possible $f(T_2)$, the distribution of the T_2 decay rate.

decay rate, and possibly width:

$$f(T_2) = \sum_m^{j-k} a_m \delta(T_2 m - T_2) + \sum_n^k a_n \frac{1}{\sqrt{2\pi}(\text{width})^2} \cdot e^{-\frac{(T_{2n}-T_2)^2}{2(\text{width})^2}}$$

A possible T_2 distribution is given in Figure (2).

- Polynomial components may exist, and their amplitudes are not known.
- The third term, an Alternating-Echo-Refocusing (AER) exists, its amplitude not known.

So, our models can be arranged in a 3-D model space. Model M_{jkl} will have

- **j** Decaying components. We assume no more than 7 such components.
- **k** Decaying components with wide distribution of the decay rate.
- **l** Polynomial components. We assume no more than 3 such components.

2.2.2 Noise

The noise, in the Bayesian interpretation, is not a ‘random’ process, but merely a process where our ignorance regarding the producing mechanism is such that its effect on the data can not be anticipated exactly. Any known behaviour of the producing mechanism can, in principle, be extracted from the noise and incorporated into the model. The noise will include any effects, systematic or not, that are present in the data but not in the model. The non-systematic effects in our case, are expected to be of finite variance but are otherwise not known. Accordingly, we assign the noise a Gaussian distribution with unknown variance[8].

2.2.3 Prior Information

We assume no preference to any model in the model space, and ignorance regarding the values of the models' parameters. The numerical representation of this ignorance is assigned by considering the amplitudes of any of our base functions as location parameters (leading to flat priors), and the decay rates and widths of components as scale parameters (leading to Jeffreys' priors). One may argue that the ignorance regarding some of the parameters should be represented differently; nonetheless, as long as we keep our priors uninformative, the influence of our ignorance representation on the final results is negligible.

The priors for all the models are assigned equal, by indifference.

2.3 The Questions

The questions we ask are always regarding the posterior probability (or *pdf*) of the proposition we are interested in.

2.3.1 Model Selection and Parameter Estimation

For each tissue, which model M_{jkl} has the highest posterior probability $p(M_{jkl}/D_{tissue}I)$? Given that model, what are the most probable values of the models' parameters?

2.3.2 Classification

After inferring about the T_2 distribution of each of the tissues, using a collection of data sets, we are interested in the following question: Given a new set of data d_{new} , we want to find the tissue it came from. We are looking for the tissue i that will maximize the probability $p(C_i/d_{new}D_iI)$ where $C_i \equiv$ "The new data was produced by the same mechanism that produced the old data set D_i ." This mechanism is described by a model (a functional form) and values of the model parameters.

2.4 The Process: Model Selection and Parameter Estimation

Section (2.2.1) defined the set of models to be tested. However, we do not wish to calculate the needed posterior probability $p(M_{jkl}/DI)$ for all these models. Though their number is finite, the computation time needed for computing all of them will render our task impractical. Our algorithm computation time is polynomial in the number of linear parameters and exponential in the number of nonlinear parameters¹. We need to find the most probable model without

¹This is since the number of linear parameters determines the dimension of matrices to be diagonalized, and the number of nonlinear parameters, on the other hand, determines the dimension of space to be searched.

Figure 3: Search Path Flow Chart. The algorithm is looking for the maximum probability in the space of models.

calculating all the models, and in particular we want to avoid unnecessary computations of models with many nonlinear parameters. In order to achieve that, we describe our model space as 3-D discrete space, using the j,k,l coordinates defined in Section (2.2.1), and search this space for the most probable model.

A flow chart of the search path is given in Figure (3), and the model space with example of search in it is given in Figure (4).

We now turn to the more detailed computation of each model. The posterior probability of model M_{jkl} is given by:

$$p(M_{jkl}/D_i I) = \int \int p(M_{jkl} \Theta_{jkl} \Phi_{jkl} / d_i I) d\Theta_{jkl} d\Phi_{jkl} \quad (4)$$

$$\propto \int \int p(d_i / M_{jkl} \Theta_{jkl} \Phi_{jkl} I) d\Theta_{jkl} d\Phi_{jkl}$$

Where Θ_{jkl} and Φ_{jkl} are the linear and nonlinear parameter sets of model M_{jkl} , respectively.

We use the formulation of Bretthorst[1]: The integration over the linear parameters is done via an orhtogonalizing transformation of the base functions. This transformation depends on the nonlinear parameters.

In order to integrate over the non-linear parameters by quadratic approximation, we transform the non-linear parameters to a new set of parameters in which the Log[likelihood] is sufficiently quadratic around its peak. In our case, this transformation is the logarithm (Figure (5)).

In Figure (6) we bring a sample of the results of applying Equation (4) to the data collected from different tissues. The figure shows the models that had been

Figure 4: Search in the Space of Models. The second-best model is not necessarily a neighbour of the best model.

selected for particular tissues and the estimated parameters for these tissues. The search for the models always started from a simple model of one decaying exponent. The credible regions for the parameters cannot be seen in the figure.

2.5 The Process: Classification

The posterior probability of C_i is just the summation, over all possible models (and the values of their parameters), of the likelihood of the model (and the values of its parameters) in light of the new data, weighted by the probability of that model (and the values of its parameters) given the old data set D_{tissue} :

$$p(C_i/d_{new}D_{tissue}I) \\ \propto \sum_{jkl} \int \int p(M_{jkl}\Theta_{jkl}\Phi_{jkl}/D_{tissue}I) \cdot p(d_{new}/\Theta_{jkl}\Phi_{jkl}M_{jkl}I) d\Theta_{jkl} d\Phi_{jkl}$$

We use Equation (2.5) to classify each pixel in a 32-image-set, generating a synthetic image, in which different classified tissues are represented by different grey levels (Figure (7)).

2.6 Discussion

2.6.1 Search in a multi-dimensional model space

In order to efficiently find the most probable model, avoiding unnecessary computation of complex models, we formulated a search routine in a 3-D model space, including stopping conditions. The arrangement of the models into the particular was not forced by the nature of the problem and is a matter of decision. The search routine used in this work found to be robust for the T_2 problem as formulated, but is definitely an *ad-hoc* development. The general problem of establishing a search routine in the model space is difficult. It is not clear what transformation should be used in order to simplify the topology and avoid many local maxima, as demonstrated in Figure (4). This transformation will in general depend on the priors of the models, the priors for the parameters values, the structure of the data, and the initial model attributes that span the space.

2.6.2 Integration over nonlinear parameters

In general, the nonlinear parameters cannot be eliminated by analytical integration, and for cases of many coupled parameters, cannot be integrated numerically either. In most cases, we have to approximate the likelihood by another function, for which analytical integration is feasible.

The normal form of the likelihood which results from the Gaussian assignment to the noise leads us to look for quadratic approximations: The behaviour of $\text{Log}[\text{Likelihood}]$ as function of any linear parameter is quadratic. In fact, the Bretthorst method for orthogonalization and integration over the linear parameters is equivalent to the integration over quadratic approximation of the function.

For the nonlinear parameters, the problem is reduced to the general problem of linear approximation; that is, finding the transformation of the nonlinear parameters that will bring the $\text{Log}[\text{likelihood}]$ to a form which is sufficiently quadratic around its peak. The transformation used in the problem of the T_2 distribution was not found in any consistent procedure, but was suggested by the nature of the specific problem as analyzed in previous, ‘frequentist’, works. The possible resulting errors in the final posterior probabilities for the models were calculated and a “safety valve routine” was applied in order to ensure detection and correction of cases in which the $\text{Log}[\text{likelihood}]$ did not transform into a quadratic enough function.

2.6.3 Noise

Our likelihood is a product of terms of the form:

$$p(d_i/\sigma\Theta\Phi I) = \frac{1}{\sqrt{2\pi\sigma_s^2}} \cdot e^{-\frac{(M_i - d_i)^2}{2\sigma_s^2}}$$

In many case we are tempted to approximate σ_s using the standard deviation of the data. We recognize that in the frame-work of probability theory as logic the ‘noise’ characterize the deviation of the individual data points from model and not from the mean of the data as the STD does. Nevertheless, assuming our model is close enough to the data mean, we hope it will serve as a sufficient approximation.

Alas, *In the case of multiple measurements, σ_s does not characterize the deviation of the individual data points from our model (“The Noise Level”)*. In the case of systematic effects not accounted for by the model, the estimation of σ_s will diverge in the limit of many measurements. In this limit, the quantity $\frac{\sigma_s}{\sqrt{n}}$ (assigned the symbol σ in this work) will converge to a finite number, characterizing the magnitude of the systematic effects in the data not accounted for by the model.

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Figure 5: Transformation of the Log[Likelihood] into Quadratic Form.

Figure 6: Results of Model Selection and Parameter Estimation for White Matter Tissues (left) and Gray Matter Tissues (right).

Figure 7: Results of Classification: The MRI Image (left) and the Classified Synthetic Image (right). Each gray level in the Synthetic Image corresponds to certain tissue. In the data used for this work, the variance among humans was larger than the difference between tissues. The resulting image fails to classify closely behaving tissues, though the discrimination between White and Gray Matter is reasonable.